

Organocatalyzed Beckmann Rearrangement of Cyclohexanone Oxime by Trifluoroacetic Anhydride in Microreactors

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Abstract

The kinetics of the Beckmann rearrangement of cyclohexanone oxime (CHO) catalyzed by trifluoroacetic anhydride (TFAA) and trifluoroacetic acid (TFA) is proposed in this work. The effects of experimental parameters on the reaction rate are studied in microreactors, including CHO concentration, TFAA concentration, temperature, and caprolactam (CPL) concentration. The reaction is verified as first-order and the reaction rate shows a linear relationship with TFAA concentration and decreases with the increasing of CPL concentration. The in-situ FTIR is adopted to study the reaction mechanism and quantitative equilibrium relationship of CPL with TFAA. Based on the experimental results, a reaction mechanism is proposed and a kinetics model is established, which is in good agreement with the experimental data. The TFAA/TFA catalytic system allows high conversion and reaction rate compared with other organic acids.

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